**Pseudoknot Molprobity Assignment**

**Objective**

The purpose of this assignment is to help Mike and Dr. B. sort through 1000 Pseudoknot structures. Each student will only need to help with 28 structures. To do this we will be using a website called **Molprobity**. This site analyzes different virtual structures and determines how effective and possible the structures are.

**What to do**

* Open up the VDS Wikispaces and click the link to the Pseudoknot Project
* Click the Google link to view the list of structures
  + <https://docs.google.com/open?id=0B_Gl3lMyhDsoYTEyNzJhMWEtMDA2Ny00Y2U3LTgzM2ItZWE1MTlmNjM4MmUz>
* Find assigned structures and download
* Go to : <http://molprobity.biochem.duke.edu/>
* On the **Browse** button - go find your .pdb file.
* Hit ' **Upload**'
* You will see a short page of some results and hopefully see an image on the right hand side (rhs), hit '**Continue**'
* Analyze all-atom contacts and geometry
* Use defaults that are already selected --> '**Run programs to perform these analyses'**
* Log in to the vdsclass google docs
* Input Data in to the Gdocs spreadsheet under the folder VDS Biooproject:
  + **All-Atom** **Contacts**
    - Clashscore, all atoms
    - percentile
  + **Nucleic Acid**  
    **Geometry**
    - Probably wrong sugar puckers
    - Bad backbone conformations
    - Residues with bad bonds
    - Residues with bad angles
* Go back to the Molprobity and Click **'Multi-criterion chart'**
* To save a copy of the page, in your web browser go to File >> Save As >> Web Page complete
* give it a name that corresponds to the structure you have analyzed. For example: **structure-0016.htm**
* Save this file to your desktop
* Repeat the above steps for each structure
* You will need to open a new Molprobity for each structure
* Upload files to the vdsclass google docs

Your assigned structures:



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